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Plastic Deformation Patterns on Cleavage Surfaces of Lithium Fluoride

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ABSTRACT

A detailed study of plastic deformation patterns on cleavage surfaces of lithium fluoride has been made by x-ray topography and optical microscopy. The nature of the deformation and some of the factors governing its generation are discussed. In particular, the presence of large cleavage steps is revealed as an important factor determining whether or not plastic relaxation will accompany cleavage. The precise manner in which cleavage proceeds is interpreted in the light of this evidence.

§ 1. INTRODUCTION

IN ionic crystals the propagation of a cleavage crack can be markedly influenced by plastic deformation generated near its tip. The extent of the deformation depends on the conditions of cleavage; for example, Gilman *et al.* (1958) observe it in lithium fluoride only when the cleavage velocity falls below a critical value ($\sim 10^{-2} \times$ longitudinal velocity of sound). Any plastic relaxation of the elastic strain energy concentrated at the crack-tip will retard the motion of the advancing crack-front. If the cleavage chisel is assumed to enter the crystal at a uniform rate the stress around the retarded crack-tip will soon build up again and cleavage will proceed until further relaxation takes place. This cyclic behaviour often leads to the appearance of discrete bands of deformation on cleavage surfaces.

Studies of the detailed structure of cleavage surfaces of ionic crystals have been made by Gilman (1957), Forty (1957), Yoshimatsu and Kohra (1960), and others. The main features of these investigations are the identification of the slip systems that comprise the plastic deformation and their effect on crack propagation. Little attention has been devoted to the role played by cleavage steps. The steps invariably present on cleavage surfaces are due to interactions of the crack-front with dislocations (forming the familiar 'river' patterns) and to asymmetric entry of the cleavage chisel. Steps formed as a result of the latter are generally larger and extend the length of the surface. This paper attempts to establish the degree of correspondence between plastic deformation produced during cleavage and the presence of these steps. The observations described

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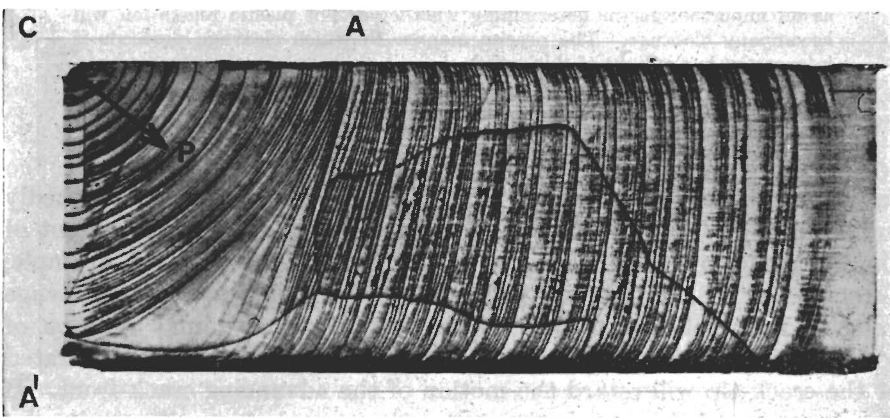
here indicate some of the factors governing the generation of the different modes of deformation.

§ 2. Experimental

Single crystals of lithium fluoride (about $15 \times 5 \times 3$ mm) were cleaved along their length. These were examined mainly by x-ray topography, although optical microscopy and etching proved useful supplementary methods. Both back-reflection topography (Newkirk 1958) and transmission topography (Lang 1957, 1959, 1963) were used with incident x-rays sufficiently collimated that only α_1 characteristic radiation contributed to the image. In all topographs shown here 'extinction contrast' (Newkirk 1958) is responsible for the diffraction contrast.

Fig. 1



Back-reflection topograph of a (100) cleavage surface of LiF, Cr Kα radiation. Reflection $\bar{2}02$. CA is along [010], CA′ along [001]. **P** is cleavage direction. Specimen length 10 mm.

A survey has been made of several cleavages, including some 'matched' surfaces. It has been found convenient to classify specimens broadly according to the velocity with which they cleaved. We thus describe 'fast' cleavages, marked by the absence of any impedance to propagation; 'slow' cleavages, which proceed in a discontinuous manner; and 'stopped' cleavages, where the crack comes to rest within the crystal. A characteristic (100) surface of a slow cleavage is shown in fig. 1. This illustrates a common feature of all specimens, namely the manner in which the crack advanced from the entry point C of the chisel. Prior to reaching AA′ its front was very nearly circular, after which it rapidly straightened out and proceeded down the length of the specimen. In the following discussion it will be found useful to consider a vector **P**, defined as a forward normal to the crack-front. It will be observed that **P** in fig. 1 may at any point be resolved into the components $\mathbf{P}_T$ and $\mathbf{P}_L$ along the transverse [001] and longitudinal

[010] directions respectively. In general, area CAA′ contained a complex pattern of gross structural distortions, slip lines, flaking of the material and other deformations. For this reason detailed attention was confined to the remainder of the cleavage surface.

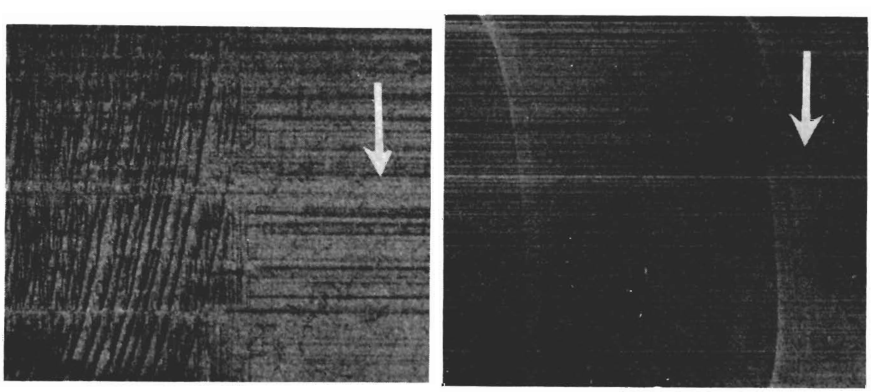
Conventional Burgers vector determinations from back-reflection topographs (220, 2$\bar{2}$0, 202, 20$\bar{2}$, 200 reflections) and transmission topographs (002, 020 reflections) confirm that the four (110) glide planes inclined at 45° to the cleavage plane are the most active during fracture. Plastic flow on two of these, the (101) and (10$\bar{1}$) planes which intersect the cleavage plane along [010], gives rise to 'longitudinal' deformation. Similarly, flow on (1$\bar{1}$0) and (110) produces 'transverse' zones of deformation along [001]. The former appear on the topographs as relatively faint, broad ribbons of diffraction contrast. They are thought to consist of dislocations wandering just below the crystal surface (Newkirk 1958). The transverse zones are seen basically as straight lines of diffraction contrast emanating from large steps. In some cases these lines aggregated to form broken arrays marking traces of the crack-front. Where the deformation was even more intense these arrays coalesced to produce the continuous dark bands shown in fig. 1. The straight-line zones are composed of adjacent dislocation half-loops, each less than 10 μm in diameter.

Details of patterns observed on individual specimens can best be described by considering the three classifications of cleavage separately.

2.1. *Fast Cleavages*

Although tranverse deformation zones were never observed in fast cleavages considerable longitudinal deformation was always evident.

Fig. 2



(*a*) (*b*)

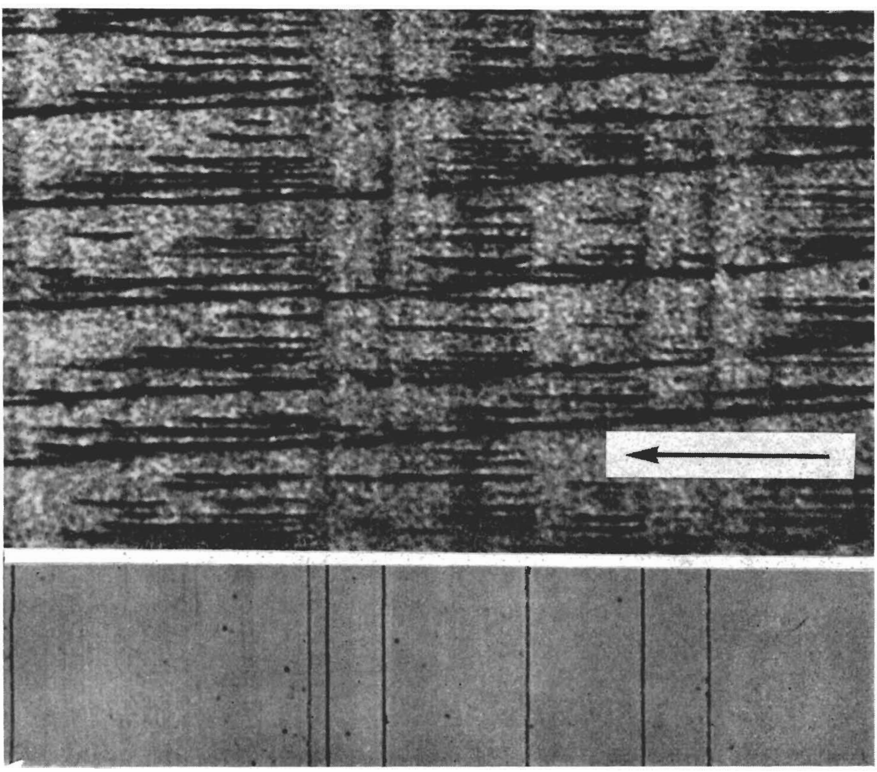
Back-reflection topographs of two cleavage surfaces. Cr Kα radiation. Reflection 202. Arrow is projection of diffraction vector onto image plane. Cleavage direction left to right. (*a*) has a few steps higher than 500 Å. Arrow length 200 μm. (*b*) has only steps smaller than 300 Å. Arrow length 400 μm.

Examination of these surfaces with an interference microscope revealed a marked absence of steps higher than about 500 Å. Figure 2 (*a*) shows an area of a cleaved crystal with a few steps exceeding this height. The crack initiated slowly and then propagated rapidly to complete the cleavage. The boundary between the two regions of different crack velocity is marked by a change in deformation pattern. It is clear that the longitudinal mode of deformation is not diminished by the increased crack velocity; it is, if anything, enhanced. It is suggested that this mode operates during all cleavages, even at crack velocities greater than Gilman's proposed critical velocity. From the width of the ribbons on the topographs it is calculated that the maximum depth of slip on these planes rarely exceeds 20 μm.

2.2. *Slow Cleavages*

At sufficiently low crack velocities there is enough time for the dislocation loops comprising the transverse zones to nucleate ahead of the crack-tip. However, not all slow cleavages showed evidence of such deformation.

Fig. 3



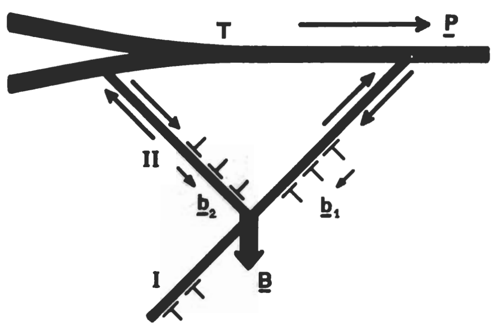
(*b*)

(*a*)

Part of cleavage surface. Cleavage direction top to bottom (*a*) Back-reflection topograph. Cr Kα radiation. Reflection 202. Arrow length 200 μm. (*b*) Optical micrograph of part of field (*a*). Magnification as for (*a*).

For instance, fig. 2 (*b*) is an area from a specimen with no steps higher than 300 Å. Although the crack has clearly halted on at least two occasions thare are no transverse zones present. Only on surfaces with steps exceeding 500 Å were they ever observed, and their density was then found to increase approximately with step height. Such a surface, with steps up to a micron high, is shown in fig. 3 (*a*), illustrating the manner in which the straight lines group into arrays and finally into extensive, continuous bands. Figure 3 (*b*), an optical micrograph of part of the same field, shows the zones to emanate from the larger steps, always in the direction opposite to that of the resolved vector $\mathbf{P}_T$. The 'sense' of steps is a further factor to be considered; the zones prefer to run into crystal on the upper side of the step. In fig. 3 (*b*) the step third from left is the only large one whose sense is unfavourable with respect to the $\mathbf{P}_T$ criterion; the density of transverse zones emanating from this step is seen to be comparatively negligible.

Fig. 4



Dislocations, Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$, interact to produce resultant **B**. Shear stresses on planes I and II arrowed. Plane of figure (001).

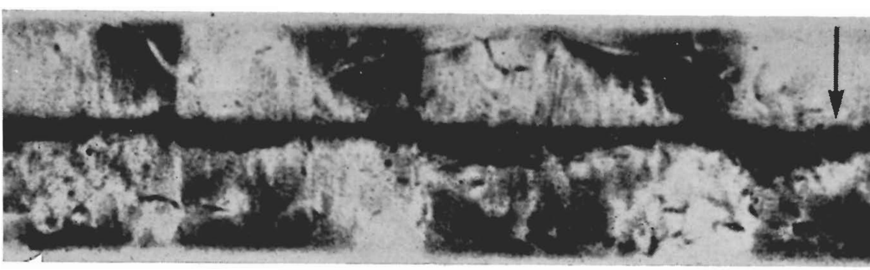
Although diffraction contrast from the transverse zone could generally be reconciled with slip on the conventional [110](1$\bar{1}$0) and [1$\bar{1}$0](110) systems (shown as $\mathbf{b}_1$(I) and $\mathbf{b}_2$(II) in fig. 4) more severely deformed specimens showed an additional contrast which could only be explained by invoking a strong [100] component of displacement. This contrast is consistent with a dislocation reaction of the type $\frac{1}{2}[110]+\frac{1}{2}[1\bar{1}0]\rightarrow[100]$. The stress distribution required to produce the reaction is shown in fig. 4. Immediately ahead of the crack-tip T shear across plane I results from tensile stress acting normally to the (100) cleavage plane. Since there are free cleavage surfaces behind T shear on plane II is due to tension parallel to the bent surfaces. This distribution of stress immediately ahead of and behind the crack-tip uniquely determines the relative sense of $\mathbf{b}_1$ and $\mathbf{b}_2$, an important factor in establishing the direction of the resultant **B**. A further, localized deformation, with component of displacement along

[001], was occasionally observed at the intersections of large cleavage steps with the more intense transverse zones. The optical micrographs showed, at these points, a tendency for the steps to be noticeably deflected along the [001] direction.

2.3. *Stopped Cleavages*

When the cleavage chisel is removed from a stopped cleavage the two cleavage surfaces tend to close near the crack-tip. The deformation patterns, apart from being more dense, were similar to those of slow cleavages. Further image contrast also arose from surface mismatch (Forty and Forwood 1963) where the two cleavage halves did not 'heal' completely. This was particularly noticeable in the neighbourhood of the larger steps, which were often some microns in height.

Fig. 5



Section topograph through stopped cleavage. MoKα radiation. Reflection 220. Arrow length 150 μm.

Since both halves of the crystal satisfy the Bragg reflecting condition simultaneously the distribution of deformation in each can conveniently be observed by taking 'section' topographs (Lang 1957). These effectively reveal a cross-sectional view of the crystal (fig. 5). The transverse zones propagate into crystal on the upper side of the steps, although cases were found in which some minor deformation occurred on the lower side. An interesting diffraction effect observed on all sections was the fan-shaped area of contrast which appeared to diverge from the deformation associated with each step. This is due to long-range elastic strain, clearly indicating the intensity of deformation in this region.

§ 3. Discussion

The experiments described in § 2 indicate the importance of cleavage steps as favourable sites for the onset of plastic relaxation during fracture. If the advancing crack-front were to be impeded and thereby distorted at a step such behaviour might be expected. In order to produce a step during cleavage, energy must be absorbed in creating the extra surface.

According to Gilman (1956) this energy, expended in the form of work required to shear material at the 'riser' of the step, will be of the order of $\frac{1}{2}Gh^2$ per unit length of step, where G is the shear modulus of the material and h is the step height. Clearly this is an overestimate, since the theoretical shear strength of perfect crystal, as derived by Mackensie (1949), yields for this energy term a value of $\frac{1}{2}(G/30)h^2$. As a result of the absorption of this additional energy a localized traction of about $\frac{1}{2}(G/30)h^2$ is exerted on the crack-front by the step. Friedel (1959) shows, for the case of a crack within an infinite solid, that this traction is accommodated by the line tension, GH^2, of the crack-front, where H is the opening of the crack at the cleavage chisel. When the dimensions of specimens used in these experiments are taken into account this line tension reduces to about $GH^2/200$, where H is typically several microns for cracks several millimetres long. Although generally $h \ll H$ the distortion of the crack-front at sufficiently high steps may lead to a significant, localized increase in stress concentration. The evidence is that a step exceeding about 500 Å in height provides a stress concentration sufficient to initiate the transverse zones of deformation.

There appears to be no reason to suspect that such a localized distortion of the crack-front would be symmetrical about a cleavage step inclined to the vector $\mathbf{P}$. Such asymmetry could well favour the initiation of the transverse zones on that side of a step away from the direction of $\mathbf{P}_T$. The effect of sense of step, on the other hand, is probably due to the distribution of shear stresses acting at the step interfaces as the cleavage halves are separated. The stresses are greatest in that part of the crystal bounded by the 'riser' of the step being created, and therefore favour slip into the upper side of the step. Taken together, these two factors imply that the patterns on matched cleavage surfaces may not necessarily be identical. While $\mathbf{P}_T$ remains unchanged the sense of the steps is reversed for each cleavage half: the topographs did in fact often reveal totally different patterns of transverse zones on matched cleavages.

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